The extreme rays of the 5×5 copositive cone

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Abstract

We give an explicit characterization of all extreme rays of the cone $\mathcal{C}_5$ of 5×5 copositive matrices. We show that the extreme rays which are not positive semi-definite or nonnegative form a 10-dimensional variety, which can be parameterized in a semi-trigonometric way.

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1. Introduction

A real symmetric $n \times n$ matrix A is called *copositive* if $x^T A x \geq 0$ for all $x \in \mathbb{R}_+^n$. The set of copositive matrices forms a convex cone $\mathcal{C}_n$, the *copositive cone*. Clearly A is copositive if it is either positive semi-definite or if all its elements are nonnegative. Hence both the cone $S_+(n)$ of all $n \times n$ real symmetric positive semi-definite matrices and the cone $\mathcal{N}_n$ of all $n \times n$ real symmetric nonnegative matrices are contained in $\mathcal{C}_n$. It is a classical result by Diananda [1] that for $n \leq 4$ the cone $\mathcal{C}_n$ equals the sum $S_+(n) + \mathcal{N}_n$. For $n \geq 5$ there exist matrices in $\mathcal{C}_n$ which cannot be represented as a sum of a positive semi-definite matrix and a nonnegative matrix. An example of such a matrix is the *Horn form* [2]

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}. \quad (1)$$

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While the sum $S_+(n)+\mathcal{N}_n$ can easily be handled algorithmically, problems involving the copositive cone are in general difficult. Of particular help in the description of the copositive cone is any information on its extreme rays. Since deciding inclusion of an integer matrix into the copositive cone is NP-complete [3], a general explicit characterization of the extreme rays of $\mathcal{C}_n$ is unlikely to be found. However, those extreme rays which belong to the sum $S_+(n)+\mathcal{N}_n$ have been characterized completely, and the Horn form (1) has been characterized as an extreme ray of $\mathcal{C}_5$ which does not belong to this sum [2]. It follows that all forms that can be obtained from the Horn form by a permutation of the indices and a scaling with a positive diagonal matrix are also extreme rays of $\mathcal{C}_5$ which do not belong to $S_+(5)+\mathcal{N}_5$.

In [4, Theorem 3.8] a procedure is presented how to construct an extreme ray of $\mathcal{C}_{n+1}$ from an extreme ray of $\mathcal{C}_n$. Those extreme rays of $\mathcal{C}_n$ with elements only from the set $\{-1,0,+1\}$ have been characterized in [5]. In [6] the dimensions of the maximal faces of the copositive and completely positive cones are studied as well as exposedness of their extreme rays. Much work has also been devoted to characterize the difference between the completely positive cone $\mathcal{C}_n^*$ and the intersection $S_+(n)\cap\mathcal{N}_n$, which are the dual cones to $\mathcal{C}_n$ and $S_+(n)+\mathcal{N}_n$, respectively. Special emphasis has been made on the 5×5 case. In [7] the extreme rays of $S_+(n)\cap\mathcal{N}_n$ for $n=5,6$ are characterized, and a procedure for general n is given. An earlier paper with a partial characterization of the 5×5 completely positive cone is [8]. In [9] extreme rays of $S_+(5)\cap\mathcal{N}_5$ which do not belong to $\mathcal{C}_5^*$ are characterized and it is shown how to separate them from $\mathcal{C}_5^*$ by a copositive matrix.

In this note we focus on the extreme rays of the cone $\mathcal{C}_5$. Baumert [10] has shown that there exist extreme rays of $\mathcal{C}_5$ which are not in the sum $S_+(5)+\mathcal{N}_5$ and are not equivalent to the Horn form in the above-mentioned sense. We use results of [10] and [11] to obtain a simple semi-trigonometric parametrization of these extreme rays, thus providing an exhaustive explicit description of all extreme rays of the cone $\mathcal{C}_5$.

1.1. Notations

For a given $n\geq 1$, denote by $e_{ij}=e_{ji}$, $i,j=1,\dots,n$, the generators of the extreme rays of the cone $\mathcal{N}_n$, normalized such that their elements are from the set $\{0,1\}$. Let e_i, $i=1,\dots,n$ be the canonical basis vectors of $\mathbb{R}^n$, and let $\Delta_n=\{x\in\mathbb{R}_+^n \mid \sum_{j=1}^n x_j=1\}$ be their convex hull.

Let $\mathrm{Aut}(\mathbb{R}_+^n)$ be the automorphism group of the positive orthant. It is generated by all $n\times n$ permutation matrices and by all $n\times n$ diagonal matrices with positive diagonal elements. This group generates a group $\mathcal{G}_n$ of automorphisms of $\mathcal{C}_n$ by $A \mapsto GAG^T$, $G \in \mathrm{Aut}(\mathbb{R}^n_+)$.

For any nonzero $x \in \mathbb{R}^n_+$, the *pattern* of x will be the vector $\mathrm{sgn}(x)^T$, where the sign function is applied elementwise.

We will work a lot with systems of equations that can be obtained from each other by a cyclical shift of indices. To simplify notation, we introduce the following index convention. The notation $k|n$ means that the index k, which can be any integer, has to be shifted modulo n into the range $1, \dots, n$. With this convention, e.g., $\psi_{6|5} := \psi_1$.

Let A be an $n \times n$ matrix, $v \in \mathbb{R}^n$ a vector, and $I \subset \{1, \dots, n\}$ a subset of indices. By A_I we denote the principal submatrix of A whose elements have row and column indices in I, and by v_I the subvector of v whose elements have indices in I. In the case $n = 5$, we define the special index sets $I^4_j = \{1, \dots, n\} \setminus \{j\}$ and $I^3_j = \{j-1|5, j, j+1|5\}$, $j = 1, \dots, 5$.

Finally, we define the 5-parametric family of matrices

$$T(\psi) = \begin{pmatrix} 1 & -\cos\psi_4 & \cos(\psi_4+\psi_5) & \cos(\psi_2+\psi_3) & -\cos\psi_3 \\ -\cos\psi_4 & 1 & -\cos\psi_5 & \cos(\psi_5+\psi_1) & \cos(\psi_3+\psi_4) \\ \cos(\psi_4+\psi_5) & -\cos\psi_5 & 1 & -\cos\psi_1 & \cos(\psi_1+\psi_2) \\ \cos(\psi_2+\psi_3) & \cos(\psi_5+\psi_1) & -\cos\psi_1 & 1 & -\cos\psi_2 \\ -\cos\psi_3 & \cos(\psi_3+\psi_4) & \cos(\psi_1+\psi_2) & -\cos\psi_2 & 1 \end{pmatrix},$$

where $\psi = (\psi_1, \dots, \psi_5)^T$ is a quintuple of angles. In various settings in the paper, these angles will satisfy one or more of the inequalities

$$\begin{aligned} \psi_j &> 0 \,\forall\, j = 1, \dots, 5, & (2) \\ \psi_j + \psi_{j+1|5} &< \pi \,\forall\, j = 1, \dots, 5, & (3) \\ \sum_{j=1}^{5} \psi_j &< \pi, & (4) \\ t_j = \cos(\psi_{j-1|5}+\psi_j+\psi_{j+1|5}) + \cos(\psi_{j-2|5}+\psi_{j+2|5}) &> 0, \,\forall\, j = 1, \dots, 5. & (5) \end{aligned}$$

2. Known results

In this section we collect known results on the structure of the cone $\mathcal{C}_n$ and its extreme rays, in particular for the value $n = 5$, which will be used later.

Theorem 2.1. *[2, Theorem 3.2] The extreme rays of $\mathcal{C}_n$ which belong to $S_+(n) + \mathcal{N}_n$ are generated by e_{ij}, $i, j = 1, \dots, n$, and by matrices of the form aa^T, where the vectors $a \in \mathbb{R}^n$ contain both positive and negative elements.*

Lemma 2.2. *[1, Lemma 7, (i)] Let $A \in \mathcal{C}_n$ be a copositive matrix, and let $x \in \mathbb{R}^n_+$ be such that $x^T A x = 0$. Let further $I = \{i \in \{1, \dots, n\} \mid x_i > 0\}$. Then A_I is positive semi-definite.*

The following slight reformulation of [10, Lemma 4.5] will be the departure point for the proof of our main result.

Lemma 2.3. *Let $A \in \mathcal{C}_5$ generate an extreme ray, and suppose that A is neither an element of the sum $S_+(5) + \mathcal{N}_5$ nor in the orbit of the Horn form (1) under the action of $\mathcal{G}_5$. Suppose further that for every pair of indices (i, j), $i, j = 1, \dots, 5$ there exists a zero $u \in \mathbb{R}^5_+$ of A with $u_i u_j > 0$. Then there exists a permutation matrix P[1] such that the set $\{x \in \Delta_5 \mid x^T P^T A P x = 0\}$ consists of 5 isolated points with patterns* $(11001), (11100), (01110), (00111), (10011)$. □

Now Theorems 5.5 and 3.1 in [11] yield the following result.

Lemma 2.4. *Let $A \in \mathcal{C}_5$ generate an extreme ray, and suppose that A is neither an element of the sum $S_+(5) + \mathcal{N}_5$. Then for every pair of indices (i, j), $i, j = 1, \dots, 5$ there exists a zero $u \in \mathbb{R}^5_+$ of A with $u_i u_j > 0$.* □

Hence the condition on the existence for every pair (i, j) of a zero u with $u_i u_j > 0$ can be omitted from Lemma 2.3, yielding the following theorem.

Theorem 2.5. *Let $A \in \mathcal{C}_5$ generate an extreme ray, and suppose that A is neither an element of the sum $S_+(5) + \mathcal{N}_5$ nor in the orbit of the Horn form (1) under the action of $\mathcal{G}_5$. Then there exists a permutation matrix P such that the set $\{x \in \Delta_5 \mid x^T P^T A P x = 0\}$ consists of 5 isolated points with patterns* $(11001), (11100), (01110), (00111), (10011)$. □

3. Main result

In this section we prove the following result.

[1] This relabeling condition has been forgotten in the original formulation of [10, Lemma 4.5].

Theorem 3.1. *Let $A \in \mathcal{C}_5$ generate an extreme ray, and suppose that A is neither an element of the sum $S_+(5) + \mathcal{N}_5$ nor in the orbit of the Horn form (1) under the action of $\mathcal{G}_5$. Then A is of the form*

$$A = P \cdot D \cdot T(\psi) \cdot D \cdot P^T, \tag{6}$$

where P is a permutation matrix, $D = \operatorname{diag}(d_1, d_2, d_3, d_4, d_5)$ with $d_j > 0$, $j = 1, \dots, 5$, and the quintuple ψ is an element of the set

$$\Phi = \{\psi \in \mathbb{R}^5 \,|\, \psi \text{ satisfies (2,4)}\}. \tag{7}$$

Conversely, for every permutation matrix P, every diagonal matrix D with positive diagonal entries, and every quintuple of angles $\psi \in \Phi$, the matrix A given by (6) generates an extreme ray of $\mathcal{C}_5$ with the above exclusion properties.

We postpone the proof of the theorem and first provide the following technical lemmas.

Lemma 3.2. *Let $C \in S_+(3)$ be such that the set $\{x \in \Delta_3 \,|\, x^T C x = 0\}$ consists of an isolated point in the interior of Δ_3. Then C can be represented in the form*

$$C = D \begin{pmatrix} 1 & -\cos\psi_1 & \cos(\psi_1+\psi_2) \\ -\cos\psi_1 & 1 & -\cos\psi_2 \\ \cos(\psi_1+\psi_2) & -\cos\psi_2 & 1 \end{pmatrix} D, \tag{8}$$

where $D = \operatorname{diag}(d_1, d_2, d_3)$ with $d_j > 0$, $j = 1, 2, 3$, and ψ_1, ψ_2 satisfy the inequalities

$$\psi_j > 0, \qquad j = 1, 2, \tag{9}$$

$$\psi_1 + \psi_2 < \pi. \tag{10}$$

Conversely, for every matrix $D = \operatorname{diag}(d_1, d_2, d_3)$ with $d_j > 0$, $j = 1, 2, 3$, and angles ψ_1, ψ_2 satisfying (9,10) the matrix C given by (8) is in $S_+(3)$ and the set $\{x \in \Delta_3 \,|\, x^T C x = 0\}$ consists of an isolated point in the interior of Δ_3, which is proportional to $D^{-1}(\sin\psi_2, \sin(\psi_1+\psi_2), \sin\psi_1)^T$.

Proof. Assume the conditions of the first part of the lemma. If C has a zero diagonal entry, say $C_{11} = 0$, then $e_1^T C e_1 = 0$, which leads to a contradiction with the assumption that the zero of C is in the interior of Δ_3. Hence the diagonal elements of C are positive. Put $d_j = \sqrt{C_{jj}}$, $j = 1, 2, 3$, and $D = \mathrm{diag}(d_1, d_2, d_3)$. If an off-diagonal element of $C' = D^{-1}CD^{-1}$ equals -1, say C'_{12}, then $(e_1 + e_2)^T C'(e_1 + e_2) = 0$, and $D^{-1}(e_1 + e_2)$ is a zero of C in $\partial\Delta_3$, again leading to a contradiction. Therefore the off-diagonal elements of C' are in the interval $(-1, 1]$, and we find angles $\psi_1, \psi_2 \in (0, \pi]$ (and hence satisfying (9)) such that $C'_{12} = -\cos\psi_1$, $C'_{23} = -\cos\psi_2$. We then have

$$\det C' = 1 + 2C'_{13}\cos\psi_1\cos\psi_2 - \cos^2\psi_1 - \cos^2\psi_2 - (C'_{13})^2 = 0,$$

which yields $C'_{13} = \cos\psi_1\cos\psi_2 + \sigma\sin\psi_1\sin\psi_2$, where $\sigma = \pm 1$. If C' is of rank 1, then $\psi_1 = \psi_2 = \pi$ and hence C' is the all-ones matrix, which contradicts the presence of a kernel vector with positive elements. Hence the rank of C' is 2 and C' has a 1-dimensional kernel, which by virtue of

$$\begin{pmatrix} 1 & -\cos\psi_1 & \cos\psi_1\cos\psi_2+\sigma\sin\psi_1\sin\psi_2 \\ -\cos\psi_1 & 1 & -\cos\psi_2 \\ \cos\psi_1\cos\psi_2+\sigma\sin\psi_1\sin\psi_2 & -\cos\psi_2 & 1 \end{pmatrix} \begin{pmatrix} \sin\psi_2 \\ \cos(\sigma(\psi_2-\frac{\pi}{2})-\psi_1) \\ -\sigma\sin\psi_1 \end{pmatrix} = 0 \qquad (11)$$

is proportional to $v_\sigma = (\sin\psi_2, \cos(\sigma(\psi_2 - \pi/2) - \psi_1), -\sigma\sin\psi_1)^T$. Note that $v_\sigma \neq 0$, since ψ_1, ψ_2 are not both equal to π. Hence v_σ has to have positive elements, which discards the choice $\sigma = 1$ and implies (10). This proves the first part of the lemma.

Let us pass to the second part. By virtue of (11) it is sufficient to show that $C' = D^{-1}CD^{-1}$ is positive semi-definite and of rank 2. This is easily seen by virtue of the factorization

$$\begin{pmatrix} 1 & -\cos\psi_1 & \cos(\psi_1+\psi_2) \\ -\cos\psi_1 & 1 & -\cos\psi_2 \\ \cos(\psi_1+\psi_2) & -\cos\psi_2 & 1 \end{pmatrix} = \begin{pmatrix} \sin\psi_1 & -\cos\psi_1 \\ 0 & 1 \\ -\sin\psi_2 & -\cos\psi_2 \end{pmatrix} \begin{pmatrix} \sin\psi_1 & -\cos\psi_1 \\ 0 & 1 \\ -\sin\psi_2 & -\cos\psi_2 \end{pmatrix}^T. \qquad (12)$$

This completes the proof. □

Lemma 3.3. *The following implications hold.*
i) (2,3,5) imply (4);
ii) (2,4) imply (3);
iii) (2–4) imply (5).

Proof. i) By (5) we have

$$\begin{aligned} \cos(\psi_{j-1|5} + \psi_j + \psi_{j+1|5}) &= -\cos\left(\left|\psi_{j-1|5} + \psi_j + \psi_{j+1|5} - \pi\right|\right) \\ &> -\cos(\psi_{j-2|5} + \psi_{j+2|5}). \end{aligned}$$

Both expressions $|\psi_{j-1|5}+\psi_j+\psi_{j+1|5}-\pi|$ and $\psi_{j-2|5}+\psi_{j+2|5}$ are contained in the interval $[0,\pi)$ by (2,3), and on this interval the cosine function is monotonely decreasing. It follows that $|\psi_{j-1|5}+\psi_j+\psi_{j+1|5}-\pi| > \psi_{j-2|5}+\psi_{j+2|5}$, which for each $j=1,\ldots,5$ amounts to the two possibilities

$$\psi_{j-1|5}+\psi_j+\psi_{j+1|5}-\psi_{j-2|5}-\psi_{j+2|5} > \pi, \qquad \sum_{j=1}^{5}\psi_j < \pi.$$

Let us prove by contradiction that the second inequality must hold. Assume that $\sum_{j=1}^5 \psi_j \geq \pi$, then for all $j=1,\ldots,5$ we have $\psi_{j-1|5}+\psi_j+\psi_{j+1|5}-\psi_{j-2|5}-\psi_{j+2|5} > \pi$. Adding all 5 inequalities together, we arrive at $\sum_{j=1}^5 \psi_j > 5\pi$, which contradicts (3). This completes the proof of i).

ii) is evident.

iii) By (2,3) we have $\psi_{j-1|5}+\psi_j+\psi_{j+1|5} > 0$ and $\psi_{j-2|5}+\psi_{j+2|5} \in (0,\pi)$, and by virtue of (4) we have $-(\psi_{j-1|5}+\psi_j+\psi_{j+1|5}-\pi) > \psi_{j-2|5}+\psi_{j+2|5} > 0$. Hence both expressions $-(\psi_{j-1|5}+\psi_j+\psi_{j+1|5}-\pi)$ and $\psi_{j-2|5}+\psi_{j+2|5}$ are in the interval $(0,\pi)$, on which the cosine function is monotonely decreasing. Thus, again by virtue of (4), we have

$$t_j = -\cos\left(\psi_{j-1|5}+\psi_j+\psi_{j+1|5}-\pi\right)+\cos(\psi_{j-2|5}+\psi_{j+2|5}) > 0,$$

yielding (5). □

Lemma 3.4. *Let* $\psi \in \mathbb{R}^5$ *satisfy (2–4). Then* $\det T(\psi) > 0$.

Proof. By Lemma 3.3,iii) we have (5). Introduce the complex variables $z_j = e^{i\psi_j}$, $j=1,\ldots,5$. We then get

$$\begin{aligned} t_j &= \frac{z_{j-1|5}z_jz_{j+1|5}+z_{j-1|5}^{-1}z_j^{-1}z_{j+1|5}^{-1}}{2}+\frac{z_{j-2|5}z_{j+2|5}+z_{j-2|5}^{-1}z_{j+2|5}^{-1}}{2} \\ &= \frac{(z_{j-1|5}z_jz_{j+1|5}+z_{j-2|5}z_{j+2|5})(1+z_1z_2z_3z_4z_5)}{2z_1z_2z_3z_4z_5}. \end{aligned}$$

This yields

$$
\begin{aligned}
\det T(\psi) &= \det \begin{pmatrix}
1 & -\frac{z_4+z_4^{-1}}{2} & \frac{z_4z_5+z_4^{-1}z_5^{-1}}{2} & \frac{z_2z_3+z_2^{-1}z_3^{-1}}{2} & -\frac{z_3-z_3^{-1}}{2} \\
-\frac{z_4-z_4^{-1}}{2} & 1 & -\frac{z_5-z_5^{-1}}{2} & \frac{z_5z_1+z_5^{-1}z_1^{-1}}{2} & \frac{z_3z_4+z_3^{-1}z_4^{-1}}{2} \\
\frac{z_4z_5+z_4^{-1}z_5^{-1}}{2} & -\frac{z_5-z_5^{-1}}{2} & 1 & -\frac{z_1-z_1^{-1}}{2} & \frac{z_1z_2+z_1^{-1}z_2^{-1}}{2} \\
\frac{z_2z_3+z_2^{-1}z_3^{-1}}{2} & \frac{z_5z_1+z_5^{-1}z_1^{-1}}{2} & -\frac{z_1-z_1^{-1}}{2} & 1 & -\frac{z_2-z_2^{-1}}{2} \\
-\frac{z_3-z_3^{-1}}{2} & \frac{z_3z_4+z_3^{-1}z_4^{-1}}{2} & \frac{z_1z_2+z_1^{-1}z_2^{-1}}{2} & -\frac{z_2-z_2^{-1}}{2} & 1
\end{pmatrix} \\
&= \frac{(1+z_1z_2z_3z_4z_5)^3 \prod_{j=1}^5 (z_{j-1|5}z_jz_{j+1|5} + z_{j-2|5}z_{j+2|5})}{16z_1^4z_2^4z_3^4z_4^4z_5^4} \\
&= t_1t_2t_3t_4t_5 \frac{2z_1z_2z_3z_4z_5}{(1+z_1z_2z_3z_4z_5)^2} = \frac{t_1t_2t_3t_4t_5}{1+\cos(\psi_1+\psi_2+\psi_3+\psi_4+\psi_5)} > 0,
\end{aligned}
$$

where the last inequality holds by $\sum_j \psi_j \in (0,\pi)$, as a consequence of (2,4), and by virtue of (5). ☐

Lemma 3.5. *Define a function $f : \Phi \to \mathbb{R}^5$ componentwise by $f_j(\psi) = -\frac{\sin\psi_j \sin(\psi_{j-2|5}+\psi_{j+2|5})}{\sin\psi_{j-1|5}\sin\psi_{j+1|5}}$, $j = 1,\ldots,5$, where Φ is given by (7). Then the equation $f(\psi) = c$, $c \in \mathbb{R}^5$ a constant vector, has only isolated solutions in Φ.*

Proof. By Lemma 3.3,ii) the elements $\psi \in \Phi$ satisfy all three sets of inequalities (2–4). The Jacobian $\frac{\partial f}{\partial\psi}$ is given by

$$
\begin{pmatrix}
-\frac{\cos\psi_1\sin(\psi_3+\psi_4)}{\sin\psi_5\sin\psi_2} & \frac{\sin\psi_1\sin(\psi_3+\psi_4)\cos\psi_2}{\sin\psi_5\sin^2\psi_2} & -\frac{\sin\psi_1\cos(\psi_3+\psi_4)}{\sin\psi_5\sin\psi_2} & -\frac{\sin\psi_1\cos(\psi_3+\psi_4)}{\sin\psi_5\sin\psi_2} & \frac{\sin\psi_1\sin(\psi_3+\psi_4)\cos\psi_5}{\sin^2\psi_5\sin\psi_2} \\
\frac{\sin\psi_2\sin(\psi_4+\psi_5)\cos\psi_1}{\sin^2\psi_1\sin\psi_3} & -\frac{\cos\psi_2\sin(\psi_4+\psi_5)}{\sin\psi_1\sin\psi_3} & \frac{\sin\psi_2\sin(\psi_4+\psi_5)\cos\psi_3}{\sin\psi_1\sin^2\psi_3} & -\frac{\sin\psi_2\cos(\psi_4+\psi_5)}{\sin\psi_1\sin\psi_3} & -\frac{\sin\psi_2\cos(\psi_4+\psi_5)}{\sin\psi_1\sin\psi_3} \\
-\frac{\sin\psi_3\cos(\psi_5+\psi_1)}{\sin\psi_2\sin\psi_4} & \frac{\sin\psi_3\sin(\psi_5+\psi_1)\cos\psi_2}{\sin^2\psi_2\sin\psi_4} & -\frac{\cos\psi_3\sin(\psi_5+\psi_1)}{\sin\psi_2\sin\psi_4} & \frac{\sin\psi_3\sin(\psi_5+\psi_1)\cos\psi_4}{\sin\psi_2\sin^2\psi_4} & -\frac{\sin\psi_3\cos(\psi_5+\psi_1)}{\sin\psi_2\sin\psi_4} \\
-\frac{\sin\psi_4\cos(\psi_1+\psi_2)}{\sin\psi_3\sin\psi_5} & -\frac{\sin\psi_4\cos(\psi_1+\psi_2)}{\sin\psi_3\sin\psi_5} & \frac{\sin\psi_4\sin(\psi_1+\psi_2)\cos\psi_3}{\sin^2\psi_3\sin\psi_5} & -\frac{\cos\psi_4\sin(\psi_1+\psi_2)}{\sin\psi_3\sin\psi_5} & \frac{\sin\psi_4\sin(\psi_1+\psi_2)\cos\psi_5}{\sin\psi_3\sin^2\psi_5} \\
\frac{\sin\psi_5\sin(\psi_2+\psi_3)\cos\psi_1}{\sin\psi_4\sin^2\psi_1} & -\frac{\sin\psi_5\cos(\psi_2+\psi_3)}{\sin\psi_4\sin\psi_1} & -\frac{\sin\psi_5\cos(\psi_2+\psi_3)}{\sin\psi_4\sin\psi_1} & \frac{\sin\psi_5\sin(\psi_2+\psi_3)\cos\psi_4}{\sin^2\psi_4\sin\psi_1} & -\frac{\cos\psi_5\sin(\psi_2+\psi_3)}{\sin\psi_4\sin\psi_1}
\end{pmatrix}.
$$

Introducing complex variables $z_j = e^{i\psi_j}$ and computing the determinant, we get

$$
\begin{aligned}
\det\frac{\partial f}{\partial\psi} &= \frac{16i(1-z_1^2z_2^2z_3^2z_4^2z_5^2)^2}{(1-z_1^2)(1-z_2^2)(1-z_3^2)(1-z_4^2)(1-z_5^2)z_1z_2z_3z_4z_5} \\
&= \frac{2\sin^2(\psi_1+\psi_2+\psi_3+\psi_4+\psi_5)}{\sin\psi_1\sin\psi_2\sin\psi_3\sin\psi_4\sin\psi_5} > 0.
\end{aligned}
$$

The last inequality comes from the fact that $\sum_{j=1}^5 \psi_j \in (0,\pi)$ by virtue of (2,4) and $\psi_j \in (0,\pi)$ by virtue of (2,3). By the implicit function theorem the function f is hence locally invertible, and its level sets consist of isolated points. $\square$

Remark 3.6. The determinants in the proofs of Lemmas 3.4 and 3.5 were computed using a computer algebra system.

In the next sections we prove Theorem 3.1.

3.1. Proof of the first part

Assume the conditions of the first part of Theorem 3.1. By Theorem 2.5 there exists a permutation matrix P such that $A = PA'P^T$ and A' has exactly 5 isolated zeros $u^1, \dots, u^5 \in \Delta_5$ with patterns (11001), (11100), (01110), (00111), (10011), respectively. Then by Lemma 2.2 the 3×3 submatrices $A'_{I_j^3}$ of A' are positive semi-definite for $j = 1, \dots, 5$. Moreover, the set $\{x \in \Delta_3 \mid x^T A'_{I_j^3} x = 0\}$ consists of a single point, namely $u^j_{I_j^3}$. Hence $A'_{I_j^3}$ satisfies the conditions of the first part of Lemma 3.2 and can be represented in the form (8). It follows that A has the structure (6) with P a permutation matrix, D a diagonal matrix with positive diagonal elements, and ψ satisfying (2,3) by virtue of (9,10). Note also that $T(\psi)$ is in the orbit of A with respect to $\mathcal{G}_5$ and hence copositive.

It remains to show inequality (4). Consider the upper left 4×4 submatrix $B = T_{I_5^4}(\psi)$ of $T(\psi)$. The matrix B is copositive and by [1, Theorem 2] must be an element of $S_+(4) + \mathcal{N}_4$, i.e., it can be represented as a sum $B' + B''$ with $B' \in S_+(4)$ and $B'' \geq 0$. By (11) the vectors $x = (\sin\psi_5, \sin(\psi_4 + \psi_5), \sin\psi_4, 0)^T$, $x' = (0, \sin\psi_1, \sin(\psi_5 + \psi_1), \sin\psi_5)^T$ are zeros of B. Since these vectors by (2,3) have nonnegative elements, they must also be zeros of both B' and B'' by the copositivity of these summands. It follows that B'' can have nonzero elements only in the upper right and lower left corners, and that both x, x' are in the kernel of B'. If, however, $B'' = 0$, then $B = B'$, and every convex combination of x, x' is also a zero of B with nonnegative elements. This contradicts the condition that A and hence $T(\psi)$ has only isolated zeros in Δ_5.

The relation $B'x = 0$ can then be rewritten as follows: there exists $t > 0$ such that

$$\begin{pmatrix} 1 & -\cos\psi_4 & \cos(\psi_4+\psi_5) & \cos(\psi_2+\psi_3)-t \\ -\cos\psi_4 & 1 & -\cos\psi_5 & \cos(\psi_5+\psi_1) \\ \cos(\psi_4+\psi_5) & -\cos\psi_5 & 1 & -\cos\psi_1 \\ \cos(\psi_2+\psi_3)-t & \cos(\psi_5+\psi_1) & -\cos\psi_1 & 1 \end{pmatrix} \begin{pmatrix} \sin\psi_5 \\ \sin(\psi_4+\psi_5) \\ \sin\psi_4 \\ 0 \end{pmatrix} = 0,$$

which yields

$$\begin{aligned} t\sin\psi_5 &= \cos(\psi_2+\psi_3)\sin\cos_5+\cos(\psi_5+\psi_1)\sin(\psi_4+\psi_5)-\cos\psi_1\sin\psi_4 \\ &= \sin\psi_5(\cos(\psi_2+\psi_3)+\cos(\psi_1+\psi_4+\psi_5)). \end{aligned}$$

Finally, by virtue of $\sin\psi_5 > 0$, which is a consequence of (2,3), we get $\cos(\psi_1+\psi_4+\psi_5) > -\cos(\psi_2+\psi_3)$. Repeating the reasoning for the other submatrices $T_{I_j^4}(\psi)$, we arrive at all of the inequalities (5). Now (4) follows from Lemma 3.3,i) and the first part of Theorem 3.1 is proven.

3.2. Proof of the second part

Assume A is as in the second part of Theorem 3.1. Since the properties of being copositive, extremal, as well as the exclusion conditions in the formulation of Theorem 3.1 are invariant under the action of $\mathcal{G}_5$, we can assume without loss of generality that both P and D are given by the identity matrix, and hence $A = T(\psi)$. Note that by Lemma 3.3 the quintuple ψ satisfies all four groups of inequalities (2–5).

3.2.1. A is copositive

The first step will be to prove copositivity of the 4×4 submatrices $A_{I_j^4}$. Let $B = T_{I_5^4}(\psi)$ as in the previous subsection. We have the representation

$$\begin{aligned} B &= \begin{pmatrix} 1 & -\cos\psi_4 & \cos(\psi_4+\psi_5) & -\cos(\psi_4+\psi_5+\psi_1)+t_5 \\ -\cos\psi_4 & 1 & -\cos\psi_5 & \cos(\psi_5+\psi_1) \\ \cos(\psi_4+\psi_5) & -\cos\psi_5 & 1 & -\cos\psi_1 \\ -\cos(\psi_4+\psi_5+\psi_1)+t_5 & \cos(\psi_5+\psi_1) & -\cos\psi_1 & 1 \end{pmatrix} \\ &= \begin{pmatrix} \sin\psi_4 & -\cos\psi_4 \\ 0 & 1 \\ -\sin\psi_5 & -\cos\psi_5 \\ \sin(\psi_1+\psi_5) & \cos(\psi_1+\psi_5) \end{pmatrix} \begin{pmatrix} \sin\psi_4 & -\cos\psi_4 \\ 0 & 1 \\ -\sin\psi_5 & -\cos\psi_5 \\ \sin(\psi_1+\psi_5) & \cos(\psi_1+\psi_5) \end{pmatrix}^T + t_5 e_{14}, \end{aligned}$$

where $t_5 = \cos(\psi_4+\psi_5+\psi_1)+\cos(\psi_2+\psi_3) > 0$ by Lemma 3.3,iii). Thus B has been represented as a sum of elements in $S_+(4)$ and $\mathcal{N}_4$. This proves copositivity of B. By repeating the argument for the other submatrices $A_{I_j^4}$, we likewise prove their copositivity.

We shall now consider the values of the quadratic form A on the compact set $C = \{x \in \mathbb{R}_+^5 \mid ||x||_2 = 1\}$. Since every 4×4 principal submatrix of A is copositive, the form A is nonnegative on the boundary of C. Thus the assumption that A is not copositive implies the existence of a local minimum x^* of the function $f(x) = x^T Ax$ in the interior of C, with $f(x^*) < 0$. This implies that x^* is an eigenvector of A with negative eigenvalue. However, by Lemma 3.4 the matrix A has at least another negative eigenvalue, and this implies the existence of a path on the shell $||x||_2 = 1$ linking x^* with $-x^*$ on which the form A is strictly negative. But since $-x^* \not\in C$, this contradicts the condition that A is nonnegative on the boundary of C. Hence A must be copositive.

3.2.2. A is extremal

From (11) it follows that A is zero on the columns $x^1, \dots, x^5$ of the matrix

$$\begin{pmatrix} \sin(\psi_3+\psi_4) & \sin\psi_5 & 0 & 0 & \sin\psi_2 \\ \sin\psi_3 & \sin(\psi_4+\psi_5) & \sin\psi_1 & 0 & 0 \\ 0 & \sin\psi_4 & \sin(\psi_5+\psi_1) & \sin\psi_2 & 0 \\ 0 & 0 & \sin\psi_5 & \sin(\psi_1+\psi_2) & \sin\psi_3 \\ \sin\psi_4 & 0 & 0 & \sin\psi_1 & \sin(\psi_2+\psi_3) \end{pmatrix}.$$

We are done if we show that A is, up to multiplication with a constant, the only copositive form that is zero on these vectors. Let B be another such form. Then the 3×3 submatrix $B_{I_j^3}$ of B is positive semi-definite by Lemma 2.2. Its kernel contains the vector $x^j_{I_j^3} = (\sin\psi_{j-2|5}, \sin(\psi_{j-2|5} + \psi_{j+2|5}), \sin\psi_{j+2|5})^T$, because $(x^j_{I_j^3})^T B_{I_j^3} x^j_{I_j^3} = (x^j)^T B x^j = 0$. Note that by virtue of (12) the submatrices $A_{I_j^3}$ have rank 2. By possibly replacing B by a convex combination $\lambda B + (1-\lambda)A$ with $\lambda > 0$ small enough, we may assume without restriction of generality that the submatrices $\lambda B_{I_j^3} + (1-\lambda)A_{I_j^3}$ also have rank 2 for all $\lambda \in [0,1]$, and their 1-dimensional kernel is generated by $x^j_{I_j^3}$.

Choose $\lambda \in [0,1]$ and set $C = \lambda B + (1-\lambda)A$. Since all elements of $x^j_{I_j^3}$ are positive, Lemma 3.2 is applicable to the submatrices $C_{I_j^3}$, and C has a representation of the form $D'T(\xi)D'$, where $D' = \mathrm{diag}(d'_1, \dots, d'_5)$ with $d'_j > 0$, $j = 1, \dots, 5$, and $\xi = (\xi_1, \dots, \xi_5)^T$ satisfies (2,3). Now by the second part of Lemma 3.2 the kernel of $C_{I_j^3}$ is proportional to the vector $(d'^{-1}_{j-1|5}\sin\xi_{j-2|5}, d'^{-1}_j \sin(\xi_{j-2|5} + \xi_{j+2|5}), d'^{-1}_{j+1|5}\sin\xi_{j+2|5})^T$. Hence there exist constants $\rho_j > 0$, $j = 1, \dots, 5$, such that for all $j = 1, \dots, 5$

$$\begin{aligned} \rho_j d'^{-1}_{j-1|5} \sin \xi_{j-2|5} &= \sin \psi_{j-2|5}, && (13) \\ \rho_j d'^{-1}_{j} \sin(\xi_{j-2|5} + \xi_{j+2|5}) &= \sin(\psi_{j-2|5} + \psi_{j+2|5}), && (14) \\ \rho_j d'^{-1}_{j+1|5} \sin \xi_{j+2|5} &= \sin \psi_{j+2|5}. && (15) \end{aligned}$$

Combining (13) for j and (15) for $j' = j + 1|5$, we obtain the relations $\rho_j d'^{-1}_{j-1|5} = \rho_{j+1|5} d'^{-1}_{j+2|5}$, $j = 1, \dots, 5$. These 5 relations determine the constants ρ_j up to a common positive factor ρ in dependence of the numbers d'_j, namely $\rho_j = \rho d'_{j-1|5} d'_j d'_{j+1|5}$. Thus (13,14) become

$$\begin{aligned} d'_{j-2|5} \rho d'_{j+2|5} \sin \xi_j &= \sin \psi_j, && (16) \\ -\rho d'_{j-1|5} d'_{j+1|5} \sin(\xi_{j-2|5} + \xi_{j+2|5}) &= -\sin(\psi_{j-2|5} + \psi_{j+2|5}). && (17) \end{aligned}$$

Multiplying on the one hand (16) with (17) for j, and on the other hand (16) for $j' = j - 1|5$ and $j'' = j + 1|5$, and taking the ratio of both products, we obtain for all $j = 1, \dots, 5$

$$-\frac{\sin \xi_j \sin(\xi_{j-2|5} + \xi_{j+2|5})}{\sin \xi_{j-1|5} \sin \xi_{j+1|5}} = -\frac{\sin \psi_j \sin(\psi_{j-2|5} + \psi_{j+2|5})}{\sin \psi_{j-1|5} \sin \psi_{j+1|5}}. \qquad (18)$$

Now note that ξ is an explicit continuous function of the elements of C, given elementwise by $\xi_j = \arccos \frac{-C_{j-2|5,j+2|5}}{\sqrt{C_{j-2|5,j-2|5} C_{j+2|5,j+2|5}}}$. For $\lambda = 0$ we have $C = A$ and hence $\xi = \psi$, which is indeed a solution of (18). Moreover, by Lemma 3.5 this is the only solution to equation (18) in some neighbourhood of ψ. Therefore $\xi \equiv \psi$ for all $\lambda \in [0, 1]$, because C is continuous in λ. From (16) we then get $d'_{j-2|5} d'_{j+2|5} = \rho^{-1}$ for all $j = 1, \dots, 5$. Taking the logarithm of these equations, we get a linear system in $\log d'_j$, whose only solution is given by $d'_j = \rho^{-1/2}$ for all $j = 1, \dots, 5$. Thus $C = \rho^{-1} A$, and B must be proportional to A. This proves the extremality of A.

3.2.3. A satisfies the exclusion properties

From (3) it follows that there exists at least one index j such that $\psi_j < \frac{\pi}{2}$. This implies $-\cos \psi_j < 0$, so $A = T(\psi)$ is not nonnegative.

Now recall that by (12) the 3×3 submatrices $A_{I_j^3}$ have rank 2. If A were positive semi-definite, it could hence not be of full rank, which contradicts Lemma 3.4.

It remains to show that A is not in the orbit of the Horn form. To see this, note that the 2×2 principal submatrices of A are of full rank by virtue of (2,3), while those of the Horn form are of rank 1, and that this property is invariant under the action of $\mathcal{G}_5$.

This completes the proof of Theorem 3.1.

4. Conclusions

Theorems 3.1, 2.1, and the fact that the Horn form is extremal in $\mathcal{C}_5$ [2] furnish an exhaustive description of the generators of the cone $\mathcal{C}_5$. While the orbit of the Horn form and the positive semi-definite extremals form 5-dimensional varieties, the extremals (6) form a 10-dimensional variety, parameterized by the diagonal elements of D and the quintuple of angles ψ. Here for each permutation P we obtain a smooth component of this variety. Since cyclic permutations of the indices and a complete reversal of order yield the same zero pattern in Theorem 2.5 and hence the same smooth component, there exist $5!/10 = 12$ such smooth components.

It is worth noting that the intersection of each smooth component with the affine subspace of matrices all whose diagonal elements equal 1 is homeomorphic to the simplex Φ given by (7). For P the identity permutation, the vertices of this simplex correspond to the Horn form (for $\psi_j = 0$ for all $j = 1, \dots, 5$) and to positive semi-definite extremals (for the other 5 vertices). The boundary points on the face opposite to the vertex $\psi = 0$ also correspond to positive semi-definite matrices (see the proof of Lemma 5.3 in [11]), while the boundary points on the other faces correspond to forms which can be represented as sums of a rank 1 PSD matrix and a matrix in the orbit of the Horn form (see [11, Theorem 3.1]).

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